Supplementary Materials

New Rod-like H-bonded Assembly Systems: Mesomorphic and Geometrical Aspects

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Characterizations

Supramolecular complex formation was confirmed by TA Instruments Co. Q20 Differential Scanning Calorimeter (DSC; USA), polarized-optical microscopy (POM, Wild, Germany) and FT-IR (Nicolet iS 10 Thermo scientific) spectroscopic analysis.

Calorimetric measurements were carried out using a PL-DSC of Polymer Laboratories, England. The instrument was calibrated for temperature, heat and heat flow according to the method recommended by Cammenga, et. al. [1]. Measurements were carried out for small samples (2–3 mg) placed in sealed aluminum pans. All measurements were conducted at a heating rate of (10 °C/min) in an inert atmosphere of nitrogen gas (10 mL/min). For DSC, the sample was heated from room temperature to 280 °C, at heating rate of 10 °C/min under nitrogen atmosphere and then cooled in the cell to 0 °C. All weighed samples were made using an ultra-microbalance, England, with accuracy ±0.0001.

Transition temperature for the 1:1 supramolecular H-bonded complexes (**An/Bm**) was investigated by DSC in heating and cooling cycles. The type of the mesophase was identified using a standard polarized-optical microscopy POM (Wild, Germany), attached with Mettler FP82HT hot stage. Measurements were made twice, and the results were found to have accuracy in transition temperature and enthalpy within ± 0.2.

Computational methods and calculations

The theoretical calculations for the investigated compounds were carried out by Gaussian 09 software [2]. DFT/B3LYP methods using 6-31G (d, p) basis set was selected for the calculations. The geometries were optimized by minimizing the energies with respect to all geometrical parameters without imposing any molecular symmetry constraints. The structures of the optimized geometries had been drawn with Gauss View [3]. Moreover, the calculated frequencies were carried out using

the same level of theory. The frequency calculations showed that all structures were stationary points in the geometry optimization method with none imaginary frequency.

References:

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